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Exam #1
October 31, 2017

CBE 100 Name [redacted]
Fundamentals of Chemical & Biomolecular Engineering Disc 1C

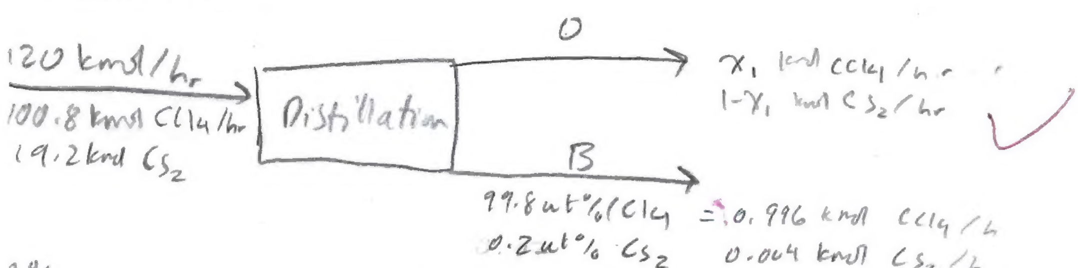
This is a 110-minute closed-book exam. Write your answers on the question sheets (you may use the back) and attach additional sheets as needed. The maximum credit for each problem is given in parentheses. The total is 100.

25

1(25). A 120 kmol/h stream containing 84 mol% carbon tetrachloride (CCl_4) and the remainder carbon disulfide (CS_2) is fed to a distillation column. Two streams exit the distillation column, an overhead stream and a bottoms stream. The overhead contains 2% of the CCl_4 entering the column. The bottoms is composed of 99.8 **wt%** CCl_4 and the remainder CS_2. Atomic weights: C, 12.01; Cl, 35.45; S, 32.06.

(a) Draw and label a flowchart.
(b) Perform a degrees of freedom analysis.
(c) Calculate the molar flow rates and molar composition of both streams exiting the distillation column.

A)



→ Convert wt% to mol%

CCl_4: $\frac{99.8\,g}{1} \times \frac{1\,mol}{153.81\,g} = 0.6489\,mol$ | mol % $\frac{0.6489}{0.6515} = 99.6\%$

CS_2: $\frac{0.2\,g}{1} \times \frac{1\,mol}{76.13\,g} = 0.002627\,mol$ | $\frac{0.002627}{0.6515} = 0.4\%$

$n_{tot} = 0.6515$

Molar Mass $CCl_4 = 12.01 + (4(35.45))$
$= 153.81\,g/mol$

$CS_2 = 12.01 + 2(32.06)$
$= 76.13\,g/mol$

B) DFA : n_{var} = 3 var (O, B, x_1)
− 2 (CCl_4, CS_2 balances)
− 1 (given information)
$\boxed{0 = DF}$

c) CCl_4 Balance
Input = Output
$100.8 = Ox_1 + 0.996B$
$100.8 = (0.02)(100.8) + 0.996B$
$\boxed{B = 99.181\,kmol/hr}$

Overall Mass Balance
$120 = O + B$
$\boxed{O = 20.819\,kmol/hr}$

Molar Flow Rates

CS_2 Balance
$19.2 = O(1-x_1) + 0.004(B)$
$19.2 = 20.819 - 20.819x_1 + 0.004(99.181)$
$\boxed{x_1 = 0.0968}$

Compositions: Overhead: 0.0968 CCl_4
0.9032 CS_2
Bottoms: 0.996 CCl_4
0.004 CS_2

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2(35). Consider a continuous, steady-state process for the production of H_2 from hexane (C_6H_{12}). However once some H_2 is formed, an undesired second reaction occurs resulting in production of ~~hexane~~ hexene (C_6H_{14}).

$$C_6H_{12} + 6H_2O \rightarrow 6CO + 12H_2 \quad (1)$$

$$C_6H_{12} + H_2 \rightarrow C_6H_{14} \quad (2)$$

In the specific process, 250 mol/h of C_6H_{12} and 800 mol/h of H_2O are fed to the reactor. The yield of H_2 is 40.0% and the selectivity of H_2 relative to C_6H_{14} is 12.0. Recall:

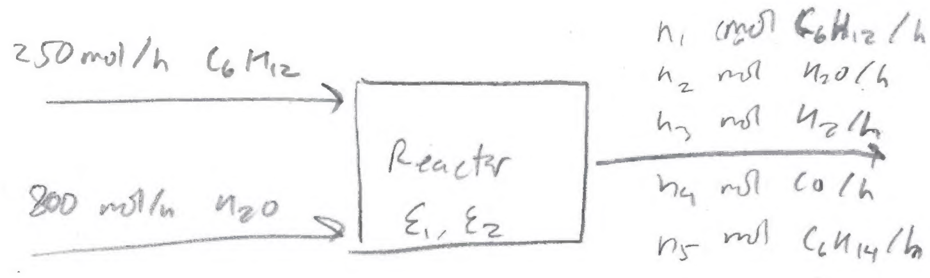
$$n_i = n_{io} + \sum_j \beta_{ij}\xi_j \qquad \begin{array}{l} i \text{ species} \\ j \text{ reaction} \end{array}$$

Yield: $\dfrac{\text{Moles of desired product formed}}{\text{Moles that would have been formed if there were no side reactions and limiting reactant had reacted completely}}$

Selectivity: $\dfrac{\text{Moles of desired product formed}}{\text{Moles of undesired product(s) formed}}$

(a) Draw and label a flowchart.
(b) Perform a degrees of freedom analysis based on mol balances.
(c) Write all the independent mol balances in terms of the ξ_j.
(d) What is the limiting reactant based on the desired reaction?
(e) Calculate the molar flow rates of all components of the output stream.
(f) Perform a degrees of freedom analysis based on *atomic* balances.
(g) Write the atomic balances on all relevant atomic species.

A)



B) DFA:

$n_{var} = 7 \; (5 \; n_1 - n_5, \; \xi_1, \xi_2)$

$n_{eqn} \; -5 \; (5 \text{ species})$

$-1 \; (\text{yield})$

$-1 \; (\text{selectivity})$

$\boxed{0} = \text{DFA}$

the rest (on attached paper)

[redacted]

① $C_6H_{12} + 6H_2O \rightarrow 6CO + 12H_2 \quad (\varepsilon_1)$

② $C_6H_{12} + H_2 \rightarrow C_6H_{14} \quad (\varepsilon_2)$

$C_6H_{12}: n_1 = 250 - \varepsilon_1 - \varepsilon_2$ ✓

$H_2O: n_2 = 800 - 6\varepsilon_1$ ✓

$H_2: n_3 = 0 - \varepsilon_2 + 12\varepsilon_1$ ✓

$CO: n_4 = 0 + 6\varepsilon_1$ ✓

$C_6H_{14}: n_5 = 0 + \varepsilon_2$ ✓

−3

D) Selectivity $= 12.0 = \dfrac{n_3}{n_5}$

$n_3 = 12 n_5$ ✓

$n_5 = \dfrac{n_3}{12}$ ✓

$n_5 = \dfrac{1200}{12} \Rightarrow \boxed{n_5 = 100 \text{ mol/hr}}$ ok.

Yield $= 0.40 = \dfrac{n_3}{\left(\dfrac{250 \text{ mol } C_6H_{12}}{1} \times \dfrac{12 \text{ mol } H_2}{1 \text{ mol } C_6H_{12}}\right)}$

$\boxed{n_3 = 1200 \text{ mol/hr}}$ −1

Find $\varepsilon_1, \varepsilon_2$

$n_5 = \varepsilon_2$

$\boxed{\varepsilon_2 = 100 \text{ mol/hr}}$ ok

$n_3 = -\varepsilon_2 + 12\varepsilon_1$

$\varepsilon_1 = \dfrac{n_3 + \varepsilon_2}{12} = \dfrac{1200 + 100}{12} = \boxed{108.3 \text{ mol/hr} = \varepsilon_1}$

Find remaining variables

$n_4 = 6\varepsilon_1$

$\boxed{n_4 = 649.8 \text{ mol/hr}}$ ok!

$n_1 = 250 - \varepsilon_1 - \varepsilon_2$

$\boxed{n_1 = 41.7 \text{ mol/hr}}$ ok.

$n_2 = 800 - 6\varepsilon_1$

$\boxed{n_2 = 150.2 \text{ mol/hr}}$ ok.

Desired reaction $= 1 \rightarrow C_6H_{12} + 6H_2O \rightarrow 6CO + 12H_2$

Ratio: $\dfrac{H_2O}{C_6H_{12}} = \dfrac{800}{250} = 3.2$

→ Theoretical Ratio $= 6$ ✓

Therefore, $\boxed{H_2O \text{ is the limiting reactant}}$

(work above)

E)

$n_1 = 41.7$ mol/hr (C_6H_{12})
$n_2 = 150.2$ mol/hr (H_2O)
$n_3 = 1200$ mol/hr (H_2)
$n_4 = 649.8$ mol/hr (CO)
$n_5 = 100$ mol/hr (C_6H_{14})

✓ ok.

[redacted]

DFA on atomic Balances

$n_{var} = 5$ (species)

$n_{eqn} = 3$ (C, H, O Balances)

-1 (selectivity)

-1 (yield)

$\boxed{0} = n_{DF}$

(ii) Atomic Balances

For C:

$$\frac{250 \text{ mol } C_6H_{12}}{h} \times \frac{6 \text{ mol C}}{1 \text{ mol } C_6H_{12}} = \frac{n_1 \text{ mol } C_6H_{12}}{h} \times \frac{6 \text{ mol C}}{1 \text{ mol } C_6H_{12}} + \frac{n_4 \text{ mol CO}}{1} \times \frac{1 \text{ mol C}}{1 \text{ mol CO}} + \frac{n_5 \text{ mol } C_6H_{14}}{1} \times \frac{6 \text{ mol C}}{1 \text{ mol } C_6H_{14}}$$

$$\Rightarrow \boxed{\frac{1500 \text{ mol C}}{hr} = 6n_1 \text{ mol C/hr} + n_4 \text{ mol C/hr} + 6n_5 \text{ mol C/hr}}$$

For H:

$$\frac{250 \text{ mol } C_6H_{12}}{hr} \times \frac{12 \text{ mol H}}{1 \text{ mol } C_6H_{12}} + \frac{800 \text{ mol } H_2O}{hr} \times \frac{2 \text{ mol H}}{1 \text{ mol } H_2O} = \frac{n_1 \text{ mol } C_6H_{12}}{1} \times \frac{12 \text{ mol H}}{1 \text{ mol } C_6H_{12}} + \frac{n_2 \text{ mol } H_2O}{1} \times \frac{2 \text{ mol}}{1 \text{ mol } H_2O} + \frac{n_3 \text{ mol } H_2}{1} \times \frac{2 \text{ mol H}}{1 \text{ mol } H_2} + \frac{n_5 \text{ mol } C_6H_{14}}{1} \times \frac{14 \text{ mol H}}{1 \text{ mol } C_6H_{14}}$$

$$\boxed{\frac{4600 \text{ mol H}}{hr} = (12n_1 + 2n_2 + 2n_3 + 14n_5) \text{ mol H/hr}}$$

For O:

$$\frac{800 \text{ mol } H_2O}{hr} \times \frac{1 \text{ mol O}}{1 \text{ mol } H_2O} = \frac{n_2 \text{ mol } H_2O}{1} \times \frac{1 \text{ mol O}}{1 \text{ mol } H_2O} + \frac{n_4 \text{ mol CO}}{1} \times \frac{1 \text{ mol O}}{1 \text{ mol CO}}$$

$$\boxed{(800 = n_2 + n_4) \text{ mol O/hr}}$$

40/40

3(40). Ethylene oxide is produced by the catalytic oxidation of ethylene:

$$2C_2H_4 + O_2 \rightarrow 2C_2H_4O \tag{1}$$

An undesired competing reaction is the combustion of ethylene:

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O \tag{2}$$

At EO Inc., the ethylene oxide production plant has undergone a major upgrade to increase production. A new reactor (R2) has been added *directly following* the old reactor (R1). The single-pass conversion of ethylene in R2 (0.25) as well as the ethylene oxide to carbon dioxide selectivity (11) are better than R1 where the corresponding values are 0.20 and 10, respectively. Downstream from the reactors, a separator generates a pure ethylene oxide product stream, a waste stream consisting solely of carbon dioxide and water, and a stream containing only ethylene and oxygen, which is recycled. This recycle stream joins with a fresh feed containing only ethylene and oxygen. The total feed to R1 is composed of ethylene and oxygen in a 3:1 ratio. EO Inc. management intends to run this plant for an ethylene oxide production rate of 1000 kmol/h. Recall that the conversion equals the amount reacted divided by the amount fed.

(a) Draw the flowchart and label it completely.
(b) Perform a degrees of freedom analysis.
(c) Assume a basis of 100 kmol/h total feed to R1 for your initial calculations and solve for all unknowns on your flowchart. For maximum credit, take a systematic approach and show all your work in a well-organized manner.
(d) Calculate the recycle and fresh feed flow rates (kmol/h) at the target ethylene oxide production rate of 1000 kmol/h.
(e) Calculate the overall ethylene conversion for the entire process and the ethylene oxide to carbon dioxide selectivity for the two-reactor sequence (R1 and R2 together).

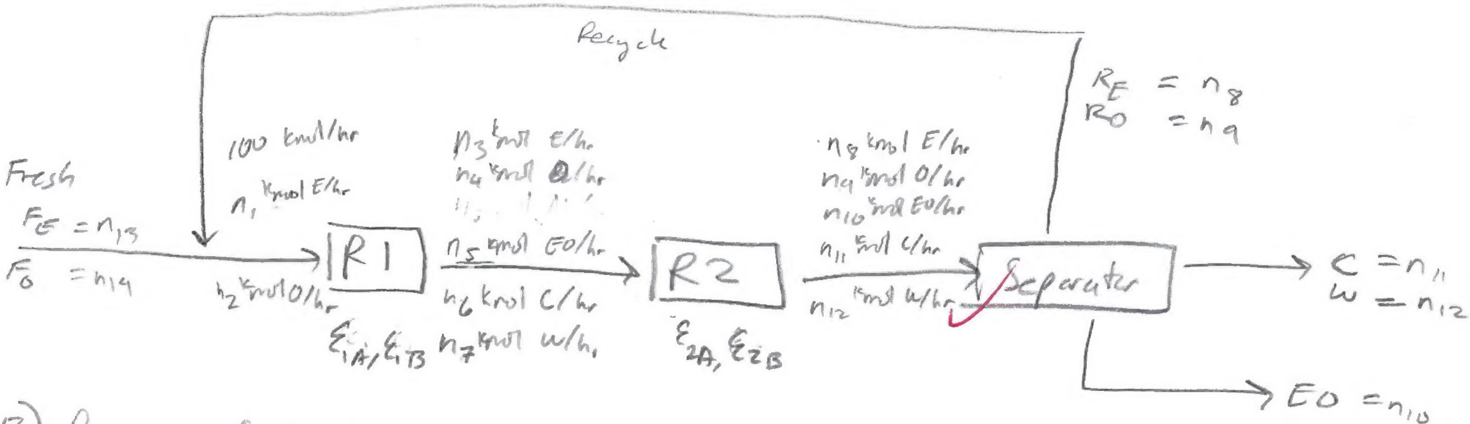
All on attached paper

[redacted]

Flow Chart: Governing Equations

$$2C_2H_4 + O_2 \rightarrow 2C_2H_4O \quad (1)$$
(E) (O) (EO)

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O \quad (2)$$
(E) (O) (C) (W)



B) Degrees of Freedom Analysis

	Mixing Point	R1	R2	Seperater	Total
n_{var}	6	9	12	5	32
n_{TIES}	−0	−2	−5	−7	−14
n_{Eqns}	−2	−5	−5	−0	−12
	4	2	2	−2	6

−2 (selectivity)
−2 (conversions)
−1 (ratio of feed)
−1 (basis)
0

C) R1 Balances

E: $n_3 = n_1 - 2\varepsilon_{1A} - \varepsilon_{1B}$

O: $n_4 = n_2 - \varepsilon_{1A} - 3\varepsilon_{1B}$

EO: $n_5 = 0 + 2\varepsilon_{1A}$

C: $n_6 = 0 + 2\varepsilon_{1B}$

W: $n_7 = 0 + 2\varepsilon_{1B}$

Selectivity: $10 = \frac{\text{mols EO}}{\text{mols C}} = \frac{n_5}{n_6} \Rightarrow n_5 = 10n_6$

Conversion: $0.20 = \frac{2\varepsilon_{1A} + \varepsilon_{1B}}{n_1} \Rightarrow 2\varepsilon_{1A} + \varepsilon_{1B} = 15$ kmol/hr

Given: 3:1 E to O; 100 kmol/hr basis
→ 0.75 E → $\boxed{n_1 = 0.75(100) = 75 \text{ kmol/hr}}$
0.25 O $\boxed{n_2 = 0.25(100) = 25 \text{ kmol/hr}}$

$n_3 = n_1 - 15$ kmol/hr → $\boxed{n_3 = 60 \text{ kmol/hr}}$

→ $2\varepsilon_{1A} + \varepsilon_{1B} = 15$ kmol/hr

$n_5 + \frac{1}{2}n_6 = 15$ kmol/hr

$10n_6 + \frac{1}{2}n_6 = 15$ kmol/hr

$\boxed{n_7 =}\ \boxed{n_6 = 1.43 \text{ kmol/hr}}$

$n_5 = 10n_6 = \boxed{14.28 \text{ kmol/hr} = n_5}$

Find $\varepsilon_{1A}, \varepsilon_{1B}$

$n_5 = 2\varepsilon_{1A}$ $\qquad$ $n_6 = 2\varepsilon_{1B}$

$\boxed{\varepsilon_{1A} = 7.14 \text{ kmol/hr}}$ $\qquad$ $\boxed{\varepsilon_{1B} = 0.714 \text{ kmol/hr}}$

Find O

$n_4 = 25 - (7.14) - 3(0.714)$

$\boxed{n_4 = 15.718 \text{ kmol/hr}}$

(cont'd) [redacted]

R2 reactor

E: $n_8 = n_3 - 2\varepsilon_{2A} - \varepsilon_{2B}$

O: $n_9 = n_4 - \varepsilon_{2A} - 3\varepsilon_{2B}$

EO: $n_{10} = n_5 + 2\varepsilon_{2A} \Rightarrow 2\varepsilon_{2A} = n_{10} - n_5$

C: $n_{11} = n_6 + 2\varepsilon_{2B} \Rightarrow \varepsilon_{2B} = \frac{n_{11} - n_6}{2}$

W: $n_{12} = n_7 + 2\varepsilon_{2B}$

Selectivity: $11 = \frac{n_{10}}{n_{11}}$

$n_{10} = 11 n_{11}$

Conversion $0.25 = \frac{2\varepsilon_{2A} + \varepsilon_{2B}}{n_3}$

$2\varepsilon_{2A} + \varepsilon_{2B} = 15$

$(n_{10} - n_5) + \left(\frac{n_{11} - n_6}{2}\right) = 15$

$(11n_{11} - n_5) + \frac{n_{11}}{2} - \frac{n_6}{2} = 15$

$11.5 n_{11} = 15 + \frac{1.43}{2} + 14.28$

$\boxed{n_{11} = 2.61 \text{ kmol/hr}}$

$\boxed{n_{10} = 28.71 \text{ kmol/hr}}$

Solve for $\varepsilon_{2A}, \varepsilon_{2B}$

$\varepsilon_{2A} = \frac{n_{10} - n_5}{2} = \frac{28.71 - 14.28}{2} = \boxed{7.215 \text{ kmol/hr}} \boxed{= \varepsilon_{2A}}$

$\varepsilon_{2B} = \frac{n_{11} - n_6}{2} = \frac{2.61 - 1.43}{2} = \boxed{0.59 \text{ kmol/hr}} \boxed{= \varepsilon_{2B}}$

Solve for n_8

$n_8 = n_3 - 2\varepsilon_{2A} - \varepsilon_{2B} = 60 - 2(7.215) - 0.59 = \boxed{44.98 \text{ kmol/hr}} \boxed{= n_8}$

$n_9 = n_4 - \varepsilon_{2A} - 3\varepsilon_{2B} = 15.718 - 7.215 - 3(0.59) = \boxed{6.733 \text{ kmol/hr}} \boxed{= n_9}$

$n_{12} = n_7 + 2\varepsilon_{2B} = 1.43 + 2(0.59) = \boxed{2.61 \text{ kmol/hr}} \boxed{= n_{12}}$

~~Separator~~

Mixing Point

E: $n_{13} + n_8 = n_1$

$n_{13} = 75 - 44.98 = \boxed{30.02 \text{ kmol/hr}} \boxed{= n_{13}}$

O: $n_{14} + n_9 = n_2$

$n_{14} = 25 - 6.733 = \boxed{14.267 \text{ kmol/hr}} \boxed{= n_{14}}$

i) Recycle: $n_8 + n_9 = 51.713$ kmol/hr

Fresh: $n_{13} + n_{14} = 48.287$ kmol/hr

EO produced: $n_{10} = 28.71$ kmol/hr

Recycle: $\frac{\text{Actual}}{\text{Mine}} = \frac{\text{Actual}}{\text{Mine}}$ (For EO) $\Rightarrow \frac{x}{51.713} = \frac{1000}{28.71}$

$\boxed{\text{Recycle} \Rightarrow x = 1801 \text{ kmol/hr}}$

Fresh $\frac{y}{48.287} = \frac{1000}{28.71}$ $\boxed{\text{Fresh} \Rightarrow y = 1681 \text{ kmol/hr}}$

E)

$$\text{Overall Ethylene Conversion} = \frac{E_{in} - E_{out}}{E_{in}} = \boxed{1}$$

$(E_{out} = 0)$ as all Ethylene is recycled.

Selectivity:

$$S_{EO/CO} = \frac{n_{10} + n_5}{n_{11} + n_6} = \frac{14.28 + 28.71}{261 + 143} = \boxed{10.64}$$